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New fingerprints of the entanglement on the thermodynamic properties

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ABSTRACT

The realization that entanglement can affect macroscopic properties of solid-state systems is a challenge in physics. Theoretical physicists often consider entanglement between the nearest neighbor spins and try to find its characteristics in terms of macroscopic thermodynamic observables. Here, we focus on the entanglement between the 2nd, 3rd, and 4th neighbor spins in an exactly solvable model. We show that there is a much clearer fingerprint of long-distance entanglement on the thermodynamic properties like specific heat, magnetocaloric effect, and magnetic susceptibility.
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چکیده

درک اینکه درهمتنیدگی می تواند بر خواص ماکروسکوپی سیستم های حالت جامد تاثیر بگذارد یک چالش در فیزیک است. فیزیکدانان دیدگاه نظری در اغلب موارد درهمتنیدگی بین نزدیکترین اسپین ها ی همسایه را در نظر گرفته و به دنبال مشخصاتی از درهمتنیدگی فوق در مشاهدهپذیرهای ماکروسکوپیک می باشند. در اینجا، ما روی درهمتنیدگی بین دومین، سومی و چهارمین همسایه ها در یک مدل دقیقا حل پذیر متمرکز می شویم. نشان می دهیم که اثر انگشت بسیار واضح تری از درهمتنیدگی بلند-فاصله روی خواص ترمودینامیکی مانند گرمای ویژه، اثر مگنتوکالریک و پذیرفتاری مغناطیسی دیده می شود.

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1 Introduction

People constantly chase to detect the predicted theoretical phenomena experimentaly. Hence, after resolving the primary challenge created about entanglement[1] by Bell inequalities[2], growing efforts were started for this goal. Although entanglement presently is not a novel phenomenon, it is still widely shrouded in mystery in the area of physics. Particularly, in three last decades, many people found that entanglement is ubiquitous in nature and it can exist in systems of any sizes and under different situations. It is a very efficient implement in teleportation, computation, and information processing tasks[3, 4, 5, 6, 7]. It still seems there are small signs of the operational research although extensive works have been done up to now. As a matter of fact, it certainly needs a prolonged route ahead. In order to achieve the technical levels, one should be able to prepare the entangled states or detect the naturally available entanglement in some compounds. The first experimental preparation report of entangled states was published by Aspect *et al*[8]. They could entangle a pair of photons. Later publications found numerous interesting applications of this phenomenon[9, 10, 11, 12]. Such developments also laid on condensed matter physics as well as quantum optics. Since particles are more convenient than photons to exchange information[4] and on the other hand, they are preferable for robust teleportation across finite distances[13, 14, 15], solids with low-dimensional structure by means of magnetic interaction between spins can be considered as channels for transferring information without the requirement for any external control[7]. The trace of entanglement has been abundantly verified in different ingredients of such magnetic solids in the microscopic world[16, 17, 18, 19]. Although there is not any straightforward approach to measure the entanglement value experimentally, but surprisingly, it has been demonstrated that it affects macroscopic properties of solids. In other words, the presence of entanglement can make a difference in the behaviour of macroscopic quantities[20]. Consequently, one can easily conclude that entanglement as a microscopic feature may reveal itself in the macroscopic world.

Some thermodynamic quantities such as magnetic susceptibility, specific heat or internal energy can distinguish an entangled state from the separable one, i. e., they are witnesses for entanglement. Investigating an entanglement witness for different low-dimensional magnets is of the central interest for both theoretical[21, 22, 23] and experimental[24, 25, 26] researches. Ghosh *et al*[24] rendered a first experimental data on the susceptibility, albeit at very low temperature (few millikelvin). In the next steps, other researches were done on different compounds in order to improve the temperature range[27, 28, 29]. For instance, based on susceptibility data for $Na_2V_3O_7$ presented by Vertesi and Bene[29], there is a critical temperature at the room temperature range where the entanglement disappears. In most compounds studied in these fields, the mentioned thermodynamic quantities are able to reveal the existence of entanglement between the nearest neighbor spins[24, 28, 29].

Nevertheless, it is an open question whether or not there are macroscopic quantities that can be as the entanglement witness for non-nearest neighbor spins. Theoretically, it was shown that magnetic susceptibility, when measured along three orthogonal spatial directions, can reveal entanglement between individual spins in a solid[30]. In a recent published paper[7], Sahling *et al* have provided an experimental realization of long-distance entanglement on $Sr_{14}Cu_{24}O_{41}$ through the magnetization and specific heat measurements. Compounds such as this dimerized chain may serve to transmit quantum information.

The main purpose of the present paper is to show whether one can find a trace of the non-nearest neighbor entanglement by studying the behaviour of some thermodynamic functions. In fact, pairwise concurrence is calculated from one-point and two-point correlation functions. As a result, it is expected that quantum phase transitions are also affected by long-distance pairwise concurrence. Here, we study what possible links there may be between them and what useful information one can extract from the behaviour of thermodynamic functions in more detail. We consider a one-dimensional (1D) spin-1/2 isotropic XY model. Solids with this type of structure have been studied both theoretically and experimentally [13, 31, 32, 33, 34] in many aspects. Since the exact energy spectrum of an infinite spin-1/2 XY chain can be obtained, one would expect a fine agreement between experience and theory. It has been already suggested that the internal energy and magnetization can be good candidates for detecting quantum entanglement in this model[35, 36]. Here, we show that the magnetic susceptibility, specific heat, and magnetocaloric effect as thermodynamic response functions can detect entanglement between the 2nd, 3rd, and 4th neighbor spins. Indeed, using the fermionization technique, we provide exact analytical expressions for entanglement between the 1st, 2nd, 3rd, and 4th neighbor spins. We show the efficiency of the thermodynamic functions in the detection of entanglement as the neighborhood of the spin pairs goes farther than the next nearest neighbor.

The paper is organized as follows. In the forthcoming section having introduced the model, we depict its Hamiltonian in spinless fermion representation. Two-point entanglement is briefly described in section 3 by introducing the concurrence and in the following it is referred to as analytical results of the concurrence between the 2nd, 3rd, and 4th neighbor spins. We present and discuss the result of our study in section 4. Investigating of three thermodynamic response functions allows us to have an analysis between their behaviour and the existence of the quantum correlations . Finally, in section 5, we will conclude and summarize our results.

2 Model

The Hamiltonian of the 1D spin-1/2 isotropic XY model in the presence of a magnetic field is given by

$$H = J\sum_{j=1}^{N}\left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y\right) - h\sum_{j=1}^{N} S_j^z, \qquad (1)$$

where $J > 0$ denotes the antiferromagnetic exchange coupling constant and h is the uniform magnetic field. This model is exactly solvable [37], and the energy spectrum has been derived by the fermionization technique[38]. This approach provides a straightforward way to obtain the exact expressions for thermodynamic quantities. By using the Jordan-Wigner transformation

$$S_j^+ = a_j^\dagger\left(e^{i\pi\sum_{l<j} a_l^\dagger a_l}\right), \qquad (2)$$

$$S_j^- = \left(e^{-i\pi\sum_{l<j} a_l^\dagger a_l}\right) a_j, \qquad (3)$$

$$S_j^z = a_j^\dagger a_j - \tfrac{1}{2}, \qquad (4)$$

and then applying the Fourier transformation, $a_j = \frac{1}{\sqrt{N}}\sum_k e^{-ikj} a_k$, the Hamiltonian can be diagonalized as follows

$$H_f = \sum_k \varepsilon(k) a_k^\dagger a_k, \qquad (5)$$

where $a_k^\dagger$ and a_k are the spinless fermionic creation and annihilation operators in the momentum space, respectively. The energy spectrum depending on the structural properties of the chain and the environment interaction is given as

$$\varepsilon(k) = J\cos(k) - h. \qquad (6)$$

3 Two-point entanglement

The pairwise concurrence, as a criteria of entanglement, is the best way to check the existence of long-range entanglement. If we adopt the Wooter's concurrence[39], we will have:

$$C(\rho_{i,i+m}) = \max\{0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}\}, \qquad (7)$$

where the λ_is are the real and non-negative eigenvalue in decreasing order of the non-Hermition matrix $R = \rho_{i,i+m}(\sigma_y \otimes \sigma_y)\rho_{i,i+m}^*(\sigma_y \otimes \sigma_y)$. σ_y is the Pauli matrix in y direction, $\rho_{i,i+m}$ is the two-particle reduced density matrix between the ith spin and its neighbor placed in the distance m as

$$\rho_{i,i+m} = \begin{pmatrix} X_{i,i+m}^+ & 0 & 0 & 0 \\ 0 & Y_{i,i+m}^+ & Z_{i,i+m}^* & 0 \\ 0 & Z_{i,i+m} & Y_{i,i+m}^- & 0 \\ 0 & 0 & 0 & X_{i,i+m}^- \end{pmatrix}, \qquad (8)$$

and finally $\rho_{i,i+m}^*$ denotes the complex conjugation of $\rho_{i,i+m}$. The concurrence in terms of $\rho_{i,i+m}$ elements is obtained as

$$C(\rho_{i,i+m}) = \max\left\{0, 2\left(|Z_{i,i+m}| - \sqrt{X^+_{i,i+m}X^-_{i,i+m}}\right)\right\}. \quad (9)$$

The reduced density matrix elements for the 1st, 2nd, 3rd, and 4th neighbor spins can be calculated as[40]

$$Z_{i,i+1} = f_1,$$
$$X^+_{i,i+1} = f_0^2 - f_1^2,$$
$$X^-_{i,i+1} = 1 - 2f_0 + f_0^2 - f_1^2, \quad (10)$$

$$Z_{i,i+2} = f_2 - 2f_0f_2 + 2f_1^2,$$
$$X^+_{i,i+2} = f_0^2 - f_2^2,$$
$$X^-_{i,i+2} = 1 - 2f_0 + f_0^2 - f_2^2, \quad (11)$$

$$Z_{i,i+3} = 4(f_1^3 - 2f_0f_1f_2 + f_2^2f_1 + f_0^2f_3 - f_1^2f_3 + f_1f_2 - f_0f_3) + f_3,$$
$$X^+_{i,i+3} = f_0^2 - f_3^2,$$
$$X^-_{i,i+3} = 1 - 2f_0 + f_0^2 - f_3^2, \quad (12)$$

$$Z_{i,i+4} = 8(f_1^4 - 3f_0f_1^2f_2 + 2f_1^2f_2^2 + 2f_0^2f_1f_3 + f_0^2f_2^2 - f_2^4 - 2f_0f_1f_2f_3 + 2f_1f_2^2f_3 - 2f_1^3f_3 + f_1^2f_3^2 - f_0f_2f_3^2 - f_0^3f_4 + 2f_0f_1^2f_4 - 2f_1^2f_2f_4 + f_0f_2^2f_4) + 4(3f_1^2f_2 - 2f_0f_2^2 - 4f_0f_1f_3 + 2f_1f_2f_3 + 3f_0^2f_4 - 2f_1^2f_4 + f_2f_3^2 - f_2^2f_4) + 2(2f_1f_3 - 3f_0f_4 + f_2^2) + f_4,$$
$$X^+_{i,i+4} = f_0^2 - f_4^2,$$
$$X^-_{i,i+4} = 1 - 2f_0 + f_0^2 - f_4^2. \quad (13)$$

It should be noted that the function f_n is defined for a non-negative integer number n as

$$f_n = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{ikn} f(k)dk. \quad (14)$$

$f(k) = \frac{1}{1+exp(\beta\varepsilon(k))}$ is the Fermi distribution function, where $\beta = 1/k_BT$ and the Boltzmann constant is taken as $k_B = 1$. The study of zero temperature entanglement of the spin-1/2 XX chain shows that for each neighbor pair of spins, there is an entanglement field, h_E[40], where the spin pair will be entangled after that. This entanglement field splits the Luttinger liquid (LL) phase into the separable and entangled regions. Also, it was reported as a function of distance m and the quantum critical field as: $h_E = \frac{(m-1)^2}{(m-1)^2+1}h_c$[40]. However, the entangled region fades away when the temperature rises. Such behaviour as a genuine quantum feature is generally not seen beyond molecular scales. As the size of the system exceeds the Avogadro constant, the decoherence interactions deteriorate the detection of quantum effects, and finally, it turns into classical phenomena. Although their own quantumness properties are not detectable, the influences are seen in some macroscopic properties known as quantum mechanical observables.

4 Results

Up to now, many works have been done to show the role of quantum correlations in the macroscopic quantities, particularly susceptibility. Many of them use the entanglement witness based on the definition of an observable that has a negative value for an entangled state[21, 41]. We apply a different approach to this purpose. Here, we are going to show that the behaviour of some thermodynamic functions can be related to the entanglement between long-distance pair spins.

The magnetic susceptibility is selected as the first candidate. Experimental results completely agree with the quantum susceptibility that is different from what is predicted by using classical correlations. It is extracted from the sum over all microscopic two-point correlation functions[42]:

$$\chi = \beta\left(\sum_{i,j=1}^{N} < S_i^z S_j^z > - < \sum_{i,j=1}^{N} S_i^z >^2\right). \qquad (15)$$

As a result, the longitudinal magnetic susceptibility is obtained as

$$\chi = \frac{\beta}{8\pi}\int_{-\pi}^{\pi}\frac{dk}{\cosh^2\frac{\beta\varepsilon(k)}{2}}. \qquad (16)$$

Figure 1 shows the magnetic field dependence of the susceptibility and the concurrence between the 1st, 2nd, 3rd, and 4th neighbor spins at a certain temperature, $T = 0.01$. Here, we recall that the quantum phase transition occurs at $h_c = J$ and the entanglement field is $h_E = \frac{(m-1)^2}{(m-1)^2+1}h_c$. In the region $h < h_c$, the ground state of the system is in the LL phase. At a quite low temperature, increasing the magnetic field gives rise to a gradual growth in the susceptibility at the first half of the LL phase. At the second half of the LL phase, by more increasing the magnetic field, the susceptibility increases rapidly and a sharp peak emerges at the near h_c which is an indication of the quantum critical point. It is believed that the mentioned peak is due to the fact that the two-point correlations, $< S_i^z S_{i+m}^z >$, will be long range in the vicinity of the quantum critical point and the correlation length becomes infinity exactly at $h = h_c$. One should note that the nonzero value of the correlation function does not necessarily imply the existence of entanglement. The entanglement contains a higher degree of correlations. To reveal it, they need to be combined in a specific way, in addition to the existence of the sufficiently strong two-point correlations, they need to be combined in a specific way. As well as two-point correlations, this kind of quantum correlations detected by concurrence has a rising behaviour in the second half of the LL region. As is seen, quantum correlations between the 2nd, 3rd, and 4th neighbor spins, in spite of the 1st neighbor spins, do not exist in the first half of the LL phase, which means that the quantum correlations cannot be long range in this region. By more increasing the magnetic field, quantum correlations between further spin pairs will be created and the amount of them increases rapidly in the second half of the LL region and shows a sharp peak similar to the susceptibility. The reason for this similarity seems simple. As we mentioned before, magnetic susceptibility includes some correlation between spins

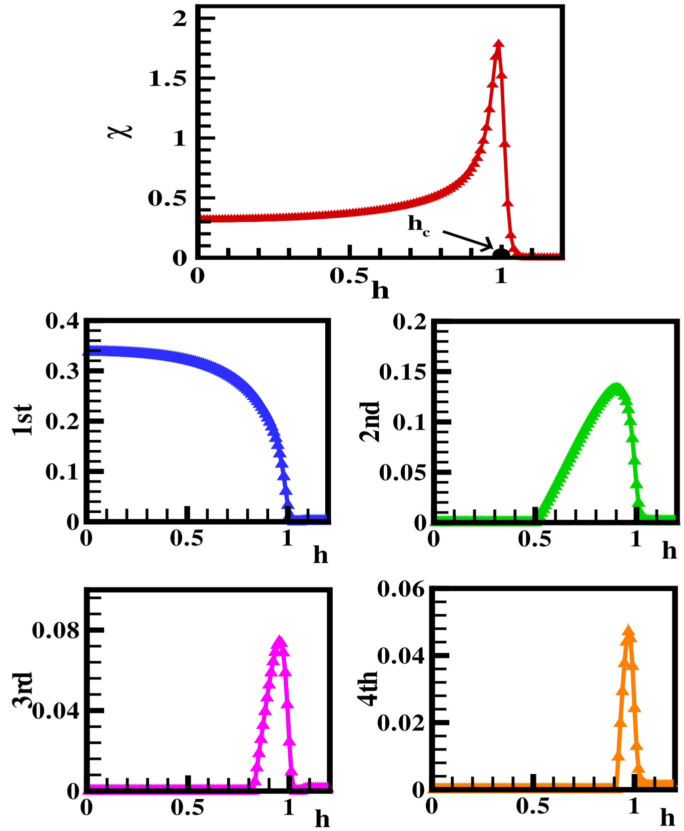

Fig. 1: (color online). The magnetic field dependence of the magnetic susceptibility (top panel) and the concurrence (bottom panels) between the 1st, 2nd, 3th, and 4th pair of spins for a chain with exchange coupling $J = 1$ at the temperature $T = 0.01$. These diagrams illustrate the roughly similar behavior for magnetic susceptibility and the concurrence between the 2nd, 3rd, and 4th spins after the entanglement field h_E.

The second bulk quantity that we are to inspect is the specific heat corresponded as variance of the Hamiltonian

$$C_v = \beta^2 k_B(< H^2 > - < H >^2), \qquad (17)$$

that we can reach to the following relation in the momentum space:

$$C_v = \frac{\beta^2 k_B}{8\pi}\int_{-\pi}^{\pi}\left(\frac{\varepsilon(k)}{\cosh\frac{\beta\varepsilon(k)}{2}}\right)^2 dk. \qquad (18)$$

The specific heat in terms of the magnetic field has two local peaks on both sides of the quantum critical point as shown in Fig. 2. It was already demonstrated that the position of the valley between two peaks is indeed the quantum critical point[44, 45]. At the considered temperature, $T = 0.01$, energy levels which are very close to the Fermi energy will be only excited. The occupation probability of these levels rises by increasing the magnetic field. As a result, two peaks are seen in the vicinity of the quantum critical field. On the other hand, the specific heat is the temperature derivative of the all two-point correlation functions between the 1st neighbor spins, $< S_i^\alpha S_{i+1}^\alpha > (\alpha = x, y, z)$. Thus, the increasing behavior of the specific heat in the second half of the LL region can be related to the increase of the temperature derivative of the correlations between the 1st neighbor spins. It is surprising that the peak of the specific heat in the second half of the LL region has very good self-identity on the cusp of the concurrence between the 2nd, 3rd, and 4th neighbor spins. According to Fig. 2, it can be argued that the increasing trend of the specific heat in the LL phase and appearance of the peak is due to the field-induced quantum correlations between the long-distance pair of spins.

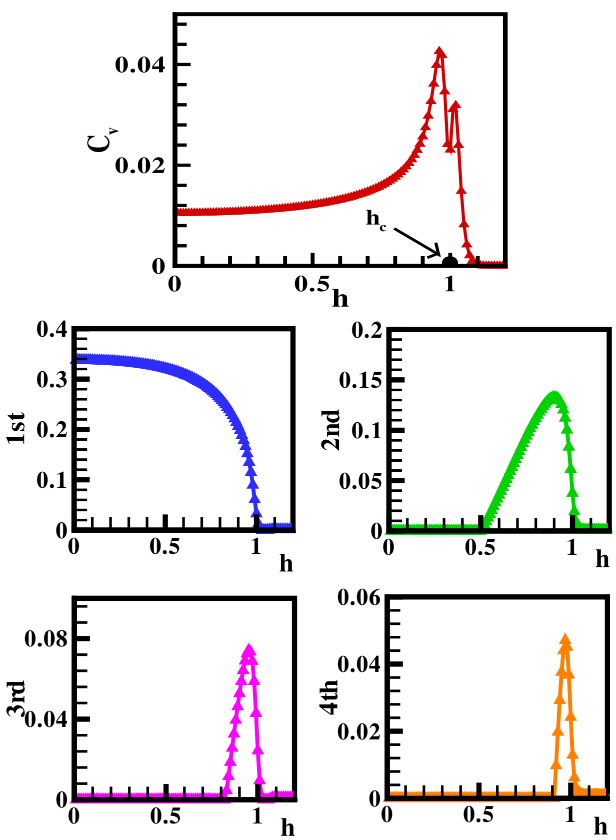

Fig. 2: (color online). The specific heat and the concurrence between 1st, 2nd, 3th, and 4th spin pairs are plotted against applied magnetic field for a chain with exchange coupling $J = 1$ at temperature $T = 0.01$ in the top and two bottom panels respectively. The figure estimates analogous trends for 2nd, 3th, and 4th concurrence and specific heat in the field range $h_E \leq h \leq h_c$.

Finally, we focus on the magnetocaloric effect which is proportional to temperature derivative of the magnetization as:

$$\Gamma = -\frac{T}{C_v}\left(\frac{\partial M}{\partial T}\right)_h. \tag{19}$$

Therefore, it can be derived from the following relation:

$$\Gamma = \frac{\beta}{8\pi C_v}\int_{-\pi}^{\pi}\frac{\varepsilon(k)}{\cosh^2\frac{\beta\varepsilon(k)}{2}}dk. \tag{20}$$

In fact, a temperature change of magnetic systems under the adiabatic variation of an external magnetic field is known as the magnetocaloric effect. This phenomenon in quantum spin systems has recently attracted scientists' attention[46]. The results for the integrated magnetocaloric and concurrence as a function of the magnetic field at the temperature $T = 0.01$ have been displayed in Fig. 3. More generally, the magnetocaloric effect is particularly large in the vicinity of the quantum critical point. It is obvious that the minimum value of the magnetocaloric expresses the quantum critical point[43]. But, what is caused maximizing the magnetocaloric is referred to as quantum correlations at the microscopic world. At first, in the absence of any entanglement between the 2nd, 3rd, and 4th neighbor spins, the magnetocaloric effect is zero. At the onset of the second half of the LL region, the rate of growth increases suddenly and both concurrence between the long-distance pair of spins and the magnetocaloric effect reach to their maximum simultaneously. However, the magnetocaloric effect plunges to its minimum while the concurrence drops smoothly to zero.

In following, we study the scaling behaviour of concurrence between the 2nd, 3rd, and 4th neighbor spins at zero temperature in the neighborhood of the entanglement field. One should note, though the concurrence does not diverge at the entanglement field, but it is affected by the quantum criticality. We analyzed our analytical results and found that as soon as the magnetic field increases from h_E, the concurrence between the 2nd, 3rd, and 4th neighbor spins increases from zero and shows a scaling behaviour as, $C \propto (h - h_E)^{\mu}$, with the critical exponent $\mu = 1.0 \pm 0.05$ for all of them. We have to mention that all concurrences show scaling behavior in the vicinity of the quantum critical field with the critical exponent $\mu = 0.33 \pm 0.01$.

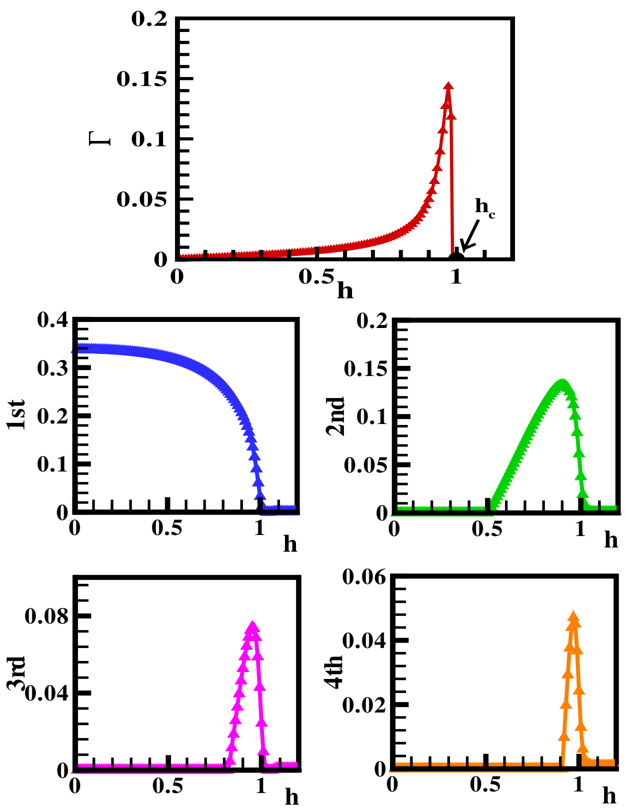

Fig. 3: (color online). Magnetocaloric in the top panel and the concurrence of the 1st, 2nd, 3th, and 4th spins in the second and third panels versus the magnetic field for a chain with exchange coupling $J = 1$ at $T = 0.01$. In the entangled region $h_E \leq h \leq h_c$, the magnetocalric adjust it's cusp to the maximum points of the quantum correlations between 2nd, 3th, and 4th spins.

5 Conclusions

In conclusion, we believe our results demonstrate that the presence of quantum entanglement between long-distance spin pairs may play a broad generic role in the macroscopic phenomena. Indeed, it is considered that an appropriate interpretation of the different behaviour of macroscopic functions observed in two halves of LL phase is due to the existence of quantum features in one of the halves. On the other hand, compounds with XY spin-1/2 structure can be treated as a transmitter of the quantum information. In fact, the 2nd, 3rd, and 4th neighbor spins must be entangled in eigenstates close to the Fermi energy. When these states contribute to the physical behaviour of the system, the fingerprint of the mentioned long-distance quantum correlations can be found in the low-temperature behaviour of the response functions.

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